



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 17, 2017 – 04:47 AM EDT

PDB ID : 5VCA
EMDB ID: : EMD-8659
Title : VCP like ATPase from T. acidophilum (VAT)-Substrate bound conformation
Authors : Ripstein, Z.A.; Huang, R.; Augustyniak, R.; Kay, L.E.; Rubinstein, J.L.
Deposited on : unknown
Resolution : 4.80 Å(reported)
Based on PDB ID : 5VC7

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

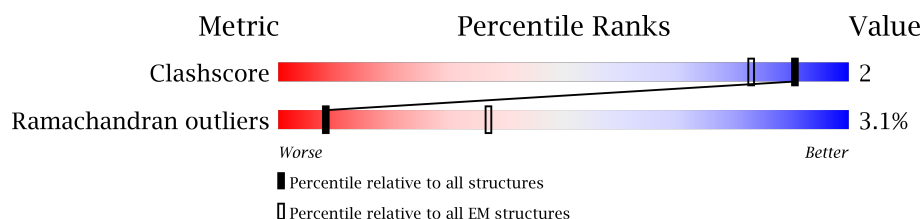
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	M	564	 91% 5% .
1	N	564	 91% 5% .
1	O	564	 91% . . .
1	P	564	 91% 5% .
1	Q	564	 91% 5% .
1	R	564	 91% 5% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VCP-like ATPase.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	P	544	Total	C	N	O	0	0
			2680	1593	544	543		
1	M	544	Total	C	N	O	0	0
			2680	1593	544	543		
1	N	544	Total	C	N	O	0	0
			2680	1593	544	543		
1	O	544	Total	C	N	O	0	0
			2680	1593	544	543		
1	Q	544	Total	C	N	O	0	0
			2680	1593	544	543		
1	R	544	Total	C	N	O	0	0
			2680	1593	544	543		

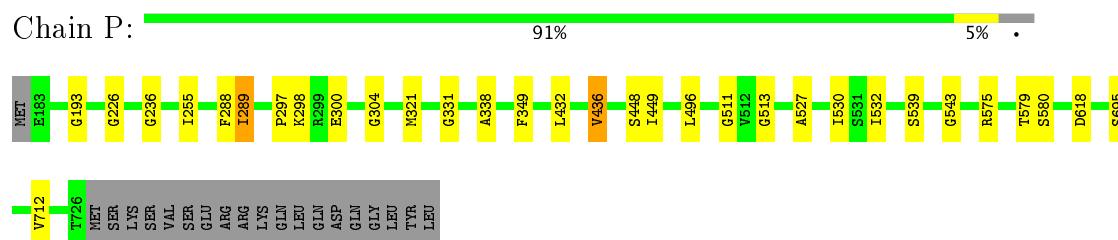
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	182	MET	-	expression tag	UNP O05209
M	182	MET	-	expression tag	UNP O05209
N	182	MET	-	expression tag	UNP O05209
O	182	MET	-	expression tag	UNP O05209
Q	182	MET	-	expression tag	UNP O05209
R	182	MET	-	expression tag	UNP O05209

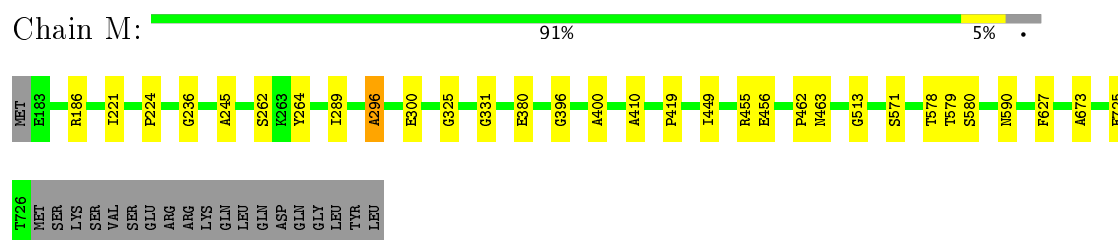
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

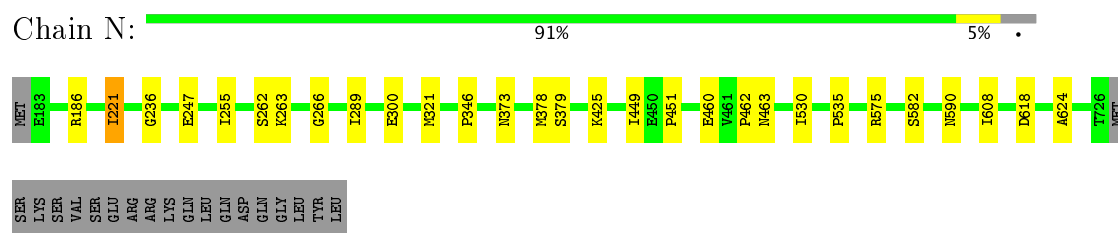
- Molecule 1: VCP-like ATPase



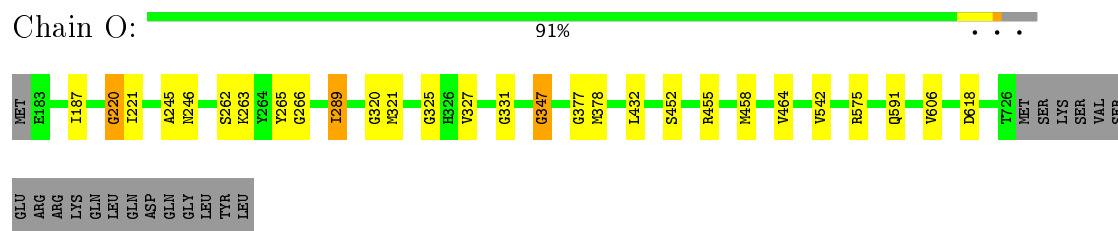
- Molecule 1: VCP-like ATPase



- Molecule 1: VCP-like ATPase



- Molecule 1: VCP-like ATPase

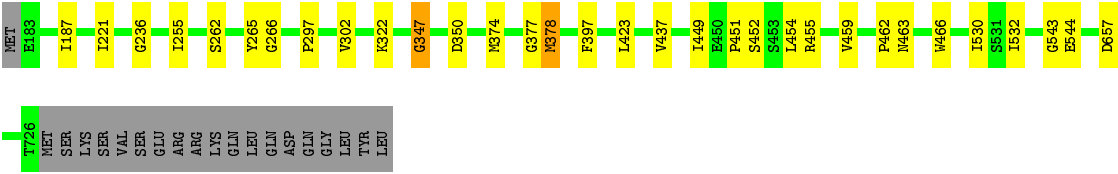


- Molecule 1: VCP-like ATPase

Chain Q:

91%

5%

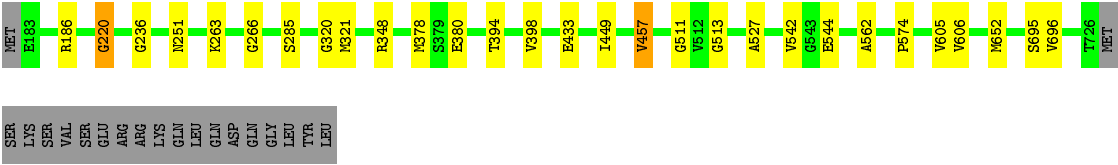


• Molecule 1: VCP-like ATPase

Chain R:

91%

5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	75205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	M	0.94	0/2679	1.18	4/3726 (0.1%)
1	N	0.99	0/2679	1.18	5/3726 (0.1%)
1	O	0.99	0/2679	1.19	4/3726 (0.1%)
1	P	0.96	0/2679	1.18	9/3726 (0.2%)
1	Q	0.98	0/2679	1.17	8/3726 (0.2%)
1	R	0.97	0/2679	1.17	6/3726 (0.2%)
All	All	0.97	0/16074	1.18	36/22356 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	457	VAL	N-CA-C	-6.81	92.61	111.00
1	P	236	GLY	N-CA-C	-6.75	96.22	113.10
1	M	396	GLY	N-CA-C	-6.58	96.65	113.10
1	M	513	GLY	N-CA-C	-6.55	96.72	113.10
1	M	296	ALA	N-CA-CB	6.44	119.11	110.10
1	P	436	VAL	N-CA-C	-5.96	94.90	111.00
1	O	347	GLY	N-CA-C	-5.94	98.26	113.10
1	M	725	GLU	N-CA-C	-5.91	95.05	111.00
1	Q	530	ILE	N-CA-C	-5.84	95.24	111.00
1	P	289	ILE	N-CA-C	-5.79	95.38	111.00
1	Q	532	ILE	N-CA-C	-5.75	95.47	111.00
1	N	255	ILE	N-CA-C	-5.74	95.49	111.00
1	Q	322	LYS	N-CA-C	-5.71	95.59	111.00
1	P	288	PHE	N-CA-C	-5.69	95.65	111.00
1	N	530	ILE	N-CA-C	-5.55	96.01	111.00
1	R	394	THR	N-CA-C	-5.54	96.04	111.00
1	R	513	GLY	N-CA-C	-5.47	99.42	113.10
1	Q	255	ILE	N-CA-C	-5.47	96.24	111.00
1	Q	466	TRP	CB-CA-C	-5.45	99.49	110.40
1	R	320	GLY	C-N-CA	5.45	135.32	121.70
1	R	695	SER	N-CA-C	-5.39	96.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	532	ILE	N-CA-C	-5.38	96.46	111.00
1	O	320	GLY	C-N-CA	5.38	135.15	121.70
1	O	289	ILE	N-CA-C	-5.36	96.53	111.00
1	P	513	GLY	N-CA-C	-5.26	99.96	113.10
1	N	449	ILE	N-CA-C	-5.25	96.82	111.00
1	R	606	VAL	N-CA-C	-5.24	96.86	111.00
1	N	289	ILE	N-CA-C	-5.22	96.91	111.00
1	P	530	ILE	N-CA-C	-5.12	97.17	111.00
1	O	606	VAL	N-CA-C	-5.10	97.22	111.00
1	P	255	ILE	N-CA-C	-5.09	97.25	111.00
1	Q	378	MET	N-CA-CB	5.08	119.75	110.60
1	Q	452	SER	N-CA-C	-5.07	97.31	111.00
1	Q	347	GLY	N-CA-C	-5.05	100.48	113.10
1	P	226	GLY	N-CA-C	-5.04	100.49	113.10
1	N	608	ILE	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	2680	0	1205	15	0
1	N	2680	0	1205	14	0
1	O	2680	0	1205	11	0
1	P	2680	0	1205	14	0
1	Q	2680	0	1205	11	0
1	R	2680	0	1205	14	0
All	All	16080	0	7230	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:262:SER:CB	1:O:266:GLY:O	1.66	1.43
1:P:579:THR:CB	1:R:542:VAL:CB	1.98	1.39
1:O:262:SER:CA	1:Q:266:GLY:HA3	1.66	1.26
1:O:262:SER:HA	1:Q:266:GLY:CA	1.62	1.25
1:P:579:THR:CB	1:R:542:VAL:HA	1.84	1.07
1:P:579:THR:CB	1:R:542:VAL:CA	2.33	1.06
1:P:539:SER:CB	1:M:590:ASN:CB	2.37	1.03
1:Q:262:SER:CB	1:R:266:GLY:O	2.08	1.02
1:Q:262:SER:HA	1:R:266:GLY:HA3	1.40	1.01
1:P:580:SER:HA	1:M:579:THR:HA	1.42	0.99
1:P:496:LEU:O	1:R:652:MET:HA	1.69	0.92
1:M:580:SER:O	1:N:582:SER:CB	2.13	0.87
1:P:580:SER:CB	1:M:578:THR:O	2.24	0.86
1:Q:262:SER:HA	1:R:266:GLY:CA	2.07	0.84
1:O:262:SER:O	1:Q:265:TYR:O	1.97	0.81
1:M:400:ALA:HB1	1:N:346:PRO:O	1.79	0.81
1:M:673:ALA:CB	1:N:624:ALA:HB3	2.16	0.75
1:P:579:THR:CA	1:R:542:VAL:CB	2.67	0.72
1:M:673:ALA:HB1	1:N:624:ALA:HB3	1.76	0.66
1:P:580:SER:HA	1:M:579:THR:CA	2.21	0.64
1:M:673:ALA:HB3	1:N:624:ALA:HB3	1.81	0.61
1:N:535:PRO:CB	1:O:591:GLN:CB	2.84	0.56
1:P:579:THR:HA	1:R:542:VAL:CB	2.37	0.55
1:O:262:SER:HA	1:Q:266:GLY:HA3	0.71	0.54
1:P:289:ILE:O	1:P:331:GLY:HA2	2.07	0.54
1:N:575:ARG:HA	1:N:618:ASP:HA	1.90	0.53
1:Q:347:GLY:H	1:Q:350:ASP:HA	1.75	0.51
1:Q:377:GLY:HA3	1:Q:437:VAL:H	1.75	0.51
1:M:262:SER:CB	1:N:266:GLY:O	2.59	0.51
1:M:289:ILE:O	1:M:331:GLY:HA2	2.13	0.48
1:N:262:SER:HA	1:O:266:GLY:HA3	1.97	0.47
1:Q:262:SER:CA	1:R:266:GLY:O	2.62	0.47
1:P:496:LEU:O	1:R:652:MET:CA	2.54	0.46
1:P:580:SER:HA	1:M:579:THR:CB	2.47	0.44
1:M:571:SER:CB	1:N:590:ASN:CB	2.95	0.44
1:M:410:ALA:CB	1:N:221:ILE:CB	2.95	0.44
1:P:575:ARG:HA	1:P:618:ASP:HA	2.00	0.44
1:R:562:ALA:O	1:R:605:VAL:HA	2.18	0.44
1:Q:374:MET:CB	1:R:220:GLY:HA2	2.48	0.43
1:O:289:ILE:O	1:O:331:GLY:HA2	2.18	0.43
1:M:673:ALA:HB1	1:N:624:ALA:CB	2.47	0.42
1:N:373:ASN:O	1:O:220:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:251:ASN:H	1:R:285:SER:HA	1.86	0.41
1:O:325:GLY:C	1:O:327:VAL:H	2.24	0.41
1:O:575:ARG:HA	1:O:618:ASP:HA	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	542/564 (96%)	482 (89%)	43 (8%)	17 (3%)	5	38
1	N	542/564 (96%)	488 (90%)	40 (7%)	14 (3%)	6	42
1	O	542/564 (96%)	489 (90%)	36 (7%)	17 (3%)	5	38
1	P	542/564 (96%)	486 (90%)	39 (7%)	17 (3%)	5	38
1	Q	542/564 (96%)	494 (91%)	30 (6%)	18 (3%)	4	37
1	R	542/564 (96%)	488 (90%)	37 (7%)	17 (3%)	5	38
All	All	3252/3384 (96%)	2927 (90%)	225 (7%)	100 (3%)	8	38

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	297	PRO
1	P	321	MET
1	P	338	ALA
1	P	449	ILE
1	P	712	VAL
1	M	449	ILE
1	M	455	ARG
1	M	456	GLU
1	M	627	PHE

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Mol	Chain	Res	Type
1	O	187	ILE
1	O	221	ILE
1	O	321	MET
1	O	378	MET
1	O	432	LEU
1	O	455	ARG
1	O	464	VAL
1	Q	221	ILE
1	Q	454	LEU
1	Q	657	ASP
1	R	321	MET
1	R	348	ARG
1	R	380	GLU
1	R	433	GLU
1	P	193	GLY
1	P	511	GLY
1	P	527	ALA
1	M	186	ARG
1	M	264	TYR
1	M	462	PRO
1	M	463	ASN
1	N	186	ARG
1	N	221	ILE
1	N	321	MET
1	N	379	SER
1	O	265	TYR
1	O	458	MET
1	O	542	VAL
1	Q	187	ILE
1	Q	297	PRO
1	Q	378	MET
1	Q	459	VAL
1	Q	463	ASN
1	Q	544	GLU
1	R	263	LYS
1	R	378	MET
1	R	511	GLY
1	R	696	VAL
1	P	298	LYS
1	P	432	LEU
1	P	695	SER
1	M	236	GLY

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Mol	Chain	Res	Type
1	N	263	LYS
1	N	300	GLU
1	N	451	PRO
1	N	460	GLU
1	O	220	GLY
1	O	245	ALA
1	O	452	SER
1	Q	236	GLY
1	Q	423	LEU
1	Q	543	GLY
1	R	527	ALA
1	R	544	GLU
1	P	300	GLU
1	M	221	ILE
1	M	296	ALA
1	M	300	GLU
1	N	236	GLY
1	N	378	MET
1	N	462	PRO
1	N	463	ASN
1	O	246	ASN
1	Q	449	ILE
1	Q	451	PRO
1	R	236	GLY
1	R	398	VAL
1	P	349	PHE
1	P	448	SER
1	M	245	ALA
1	M	380	GLU
1	N	247	GLU
1	N	425	LYS
1	Q	397	PHE
1	Q	462	PRO
1	R	186	ARG
1	R	574	PRO
1	P	304	GLY
1	M	224	PRO
1	M	325	GLY
1	O	263	LYS
1	Q	455	ARG
1	P	543	GLY
1	O	377	GLY

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Mol	Chain	Res	Type
1	R	449	ILE
1	R	457	VAL
1	R	220	GLY
1	O	347	GLY
1	Q	302	VAL
1	P	436	VAL
1	M	419	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.